FAP 9B4647

Section H. Environmental Assessment

1. **Date:** June 18, 1999

2. **Name of Petitioner:** Exxon Company International

3. **Address:** 200 Park Avenue, Florham Park, NJ 07932-1002

4. **Description of the requested action:**

a. Requested approval: The indirect food additive that is the subject of this petition is isopropyl laurate. Throughout this assessment, isopropyl laurate will be referred to as IPL. The purpose of this Food Additive Petition is to amend 21 C.F.R. §178.3910 to allow for the use of IPL in surface lubricants used in the manufacture of metallic articles intended for food contact use at a level not to exceed 10 % weight of the finished formulation. Specifically, the petition seeks to add isopropyl laurate to list (a)(2) of 21 C.F.R. §178.3910.

b. Need for action: IPL does not have a technical effect in food nor is it intended to be added directly to food. As described in this section, and in Section C of this Petition, IPL is intended to be used as a component of surface lubricants used to roll metallic foil or sheet stock. Any migration of IPL into food is incidental to the use of these surface lubricants.

The surface lubricants used to roll metallic foil or sheet stock typically consist of a mineral oil compliant with 21 C.F.R. 178.3620(c) or a light petroleum hydrocarbon as identified in 178.3910 (a)(4) as the main component, and various additives. The function of the additives is to control friction in the roll gap and to improve the oxidation stability of the lubricant. Control of friction in the roll gap is very important for the rolling process. The level of friction has a major influence on rolling speed, achievable thickness reduction per pass, and surface quality of the rolled metal.

Apart from the rolling process, the surface lubricant also plays an important role in the annealing process which is usually carried out as an intermediate step to reduce work-hardening of the rolled metal or subsequently to rolling in order to achieve certain properties of the rolled metal and/or to evaporate the remaining surface lubricant from the surface of the rolled metal. In the annealing process oils of the rolled metal are heated to a temperatures between 250 and 450 °C in an oven. The maximum temperature depends on the desired mechanical properties (e.g., hardness, tensile strength). The lack of residual surface lubricant or decomposition products on the foil after annealing is also important. For rolling of metallic aluminum foils or sheet stock, esters of straight-chain carboxylic acids as identified in, 178.3910(a) and (b) are widely used to reduce friction in the roll gap. These esters include methyl esters of fatty acids (C17 - C18) derived from animal and vegetable fats and oils, isopropyl oleate, isobutyl stearate and n-butyl stearate. These esters are effective in

99F-0459

reducing friction but have boiling points above 315 °C and tend to form brown stains during annealing. In contrast, IPL has a boiling point of 270 to 277 °C, depending on the method of measurement. Results of bench tests show that this low boiling point provides for favorable annealing behavior with minimal discoloration and no browning.

IPL is very effective in reducing friction in the roll gap. This has been demonstrated in so-called "plane compression tests" where an aluminum specimen is compressed between two steel platens, mounted in a hydraulic press. Before applying pressure, the surface of the aluminum specimen is wetted with the test surface lubricant and the thickness reduction after compression is measured. This test, which simulates the rolling process, gave for a typical hydrocarbon used as base fluid for surface lubricants without any additional substance a thickness reduction of 38%. Adding 4.1 mass% of IPL to this hydrocarbon resulted in a thickness reduction of 50% under the same test conditions. This increase in thickness reduction is a clear indication of the capability of IPL to reduce friction in the roll gap. Furthermore, IPL shows a strong synergistic effect on friction reduction with small amounts of 21 C.F.R. 178.3910(b) compliant fatty acids derived from animal and vegetable fats and oils. A test oil comprised of 95.4% of the above-mentioned hydrocarbon, 4.1% IPL, and 0.5% lauric acid gave a thickness reduction of 61% in the plane compression test.

The effective friction reducing properties of IPL combined with the high evaporative properties and very low tendency to form brown stains makes IPL superior to conventional esters in surface lubricants for rolling metallic foil or sheet stock. IPL is intended to replace higher boiling esters in the formulation of surface lubricants in order to minimize brown staining problems and to apply lower annealing temperatures.

c. Locations of use/disposal: The location where IPL will be used will be an aluminum foil manufacturing plant in Germany (the largest such plant in Europe). The design of the plant may be considered typical of European aluminum foil plants. As described in section 6 below, approximately one third of the IPL consumed at the plant will be removed via filter cakes as part of the lubricant recycling process and subsequently combusted in a cement kiln. Nearly half of the IPL throughput will be destroyed in the annealing process. Evaporative losses during rolling will be trapped in a vapor recovery system and re-distilled. The residue from re-distillation (bottoms) will be incinerated.

Food-packaging materials containing small quantities of IPL will be used in patterns corresponding to the national population density and will be widely distributed across the country. Consequently, disposal will occur nationwide with material ultimately being deposited in landfills (78%) and incinerated (22%). The food packaging materials made of metallic rolls and sheets will not be recycled to any appreciable degree.

5. Identification of substances that are the subject of the requested action:

The indirect food additive that is the subject of this petition is isopropyl laurate, the isopropyl ester of lauaric acid. IPL is identified by Chemical Abstract Service Registry Number 10233-13-3 and European Inventory of Existing Chemical Substances Number 2335601. Unichema markets IPL under the commercial name ESTOL 1505. Selected physical and chemical properties of IPL are listed below and additional information is included in the attached Material Safety Data Sheet.

Molecular Weight: 242
Molecular Formula: $C_{15}H_{30}O_2$
Structural formula: $CH_3(CH_2)_{10}COOCH(CH_3)_2$
Physical description: colorless liquid

6. Introduction of substances into the environment

a. Introduction of substances into the environment as a result of manufacture: No extraordinary circumstances apply to the manufacturing of IPL. No unique emission circumstances exist that are not otherwise adequately addressed by general or specific emission requirements including occupational requirements promulgated by Federal, State or local environmental agencies and emissions of IPL are not expected to harm the environment. No proposed actions threaten a violation of federal, state, or local environmental laws or requirements. The production of IPL is not expected to adversely affect a species or the critical habitat of a species determined under the Endangered Species Act or the Convention on International Trade in Endangered Species of Wild Fauna and Flora to be endangered or threatened, or wild fauna or flora that are entitled to special protection under any other Federal law.

b. Introduction of substances into the environment as a result of use: The application of rolling fluids during the rolling of aluminum foil or sheet stock occurs in a controlled, confined section of the mill system. The mill is equipped air wipes on the sheet passing through the mill and an effective ventilation system. The exhaust air passes through a mist removal system and a vapor recovery system (AIRPURE® system). These systems minimize the levels of rolling fluid in the workroom atmosphere and the evaporation losses. Levels of oil mists are well below applicable occupational health guidelines, Maximum Concentrations at the Workplace, or MACs, established by the Commission for the Investigation of Health Hazards of Chemical Compounds in the Work Area of the German Research Society. No specific occupational health guideline is available for IPL but the German TRGS 900 regulation for hydrocarbons would apply and that is 600 mg/m^3. In a series of exposure measurements in the rolling plant described above, using personal samplers for 4-hour intervals, exposure levels in the range of 0.8 and 1.9 mg/m^3 were found. When IPL is used as an additive in the rolling oil only a small percentage of this exposure would be to IPL.

In the plant, the rolling fluids are re-circulated in a closed system. Consequently, there should be practically no releases to water from an aluminum foil rolling plant.

The large plant described earlier consumes approximately 2200 tons/year of rolling oil fluid, of which about 1400 tons/yr. will contain IPL. The IPL will comprise about 4% (at most 10%) of the 1400 tons/yr. of oil or 56 tons/yr. of IPL. In the re-circulation system, the rolling oil fluid passes through an in-line active earth filter. This filter will be changed periodically and the spent filter cakes burned in a cement kiln, the IPL being combusted to carbon dioxide. About 450 tons of rolling, oil containing approximately 20 tons of IPL, will be consumed in this manner. Mist and vapor recovery systems remove most of the mists and vapors generated during rolling from the exhaust air from the mill. About 10% of the IPL (about 6 tons/yr.) are expected to not be recovered by these systems and be released to air. The recovered mists and vapors will be re-distilled and recycled under normal circumstances. About 650 tons of rolling oil, containing approximately 26 tons of IPL, will be consumed during the annealing process. Most of it will be completely oxidized or decomposed. The decomposition products and evaporative losses in the exhaust air from the annealing furnaces pass through a catalytic after-burner and are totally combusted. The bottoms from the re-distillation units are disposed of in special waste incinerators for production of heat/energy.

The consequence of IPL being handled in closed systems, being re-circulated, and waste streams being incinerated, is that the amount of IPL entering the environment is negligible. The only sources are small amounts passing the vapor recovery system and losses during re-distillation. These losses are likely to be about 6 tons per year. These fugitive emissions may be partly as vapor. But the low vapor pressure of IPL (see section 7) would indicate that they would condense to form aerosols. Although there are no specific air limits for IPL, the plant meets the German regulatory emission requirements under TA-LUFT applicable for oil mist (150 mg HC/m^3) and other esters (100 mg/m^3).

c. Introduction of substances into the environment as a result of disposal: The metallic food packaging material will contain a very small amount of IPL, not greater than 0.015 mg/in^2. It will not migrate from the food packaging material into landfill leachate because it has very low water solubility and will adhere strongly to organic matter. Moreover, even if a very small amount of IPL migrates from the food packaging into landfill leachate, extremely low quantities would enter the environment; based on the Environmental protection Agency's regulations governing municipal solid waste landfills.

Nearly all the throughput of the manufacturing plant is disposed of through incineration. Based on the elemental composition of IPL (C, H, and O), no significant change in incinerator emissions is expected to result from incinerating rolling oil or food-contact material containing IPL.

7. Fate of substance released into the environment:

IPL is a simple ester of a naturally occurring fatty acid (lauric) and isopropyl alcohol. Ester bonds are biologically quite degradable and all organisms possess esterase enzymes. Thus, based on structure, IPL is expected to be biodegradable. This is confirmed by computer estimation with the US EPA 'Biodegradation Probability Program' (BPP), which gives a non-linear probability result of 0.9959 (values >0.5 indicate rapid biodegradation). Abiotic hydrolysis (base catalyzed) is expected to be slow (half-life > 1 yr.) at neutral pH for such esters. The Air Oxidation Potential (AOP) computer model calculates an atmospheric half-life of 7.8 hrs.

Using the combined results of the environmental assessment programs ASTER (US EPA, Duluth) and EPIWIN (Syracuse Research Corp./US EPA), the following physical constants are estimated for IPL:

Water solubility:	0.029 mg/L
Vapor Pressure:	0.0038 mm Hg (at 32°C)
Octanol/water (log K_{ow}):	6.23

These values for physical properties may be used to model the relative partitioning behavior expected for IPL between environmental compartments if there is a hypothetical release of IPL to the environment. An equilibrium model (Mackay et al. (1996) level I, EQC Model v. 1.0), which assumes no degradation in the environment, gives the following predicted environmental distributions:

Air	0.416%
Soil	97.3%
Sediment	2.162%
Water	0.065%
Suspended sediment	0.068%

IPL is used in metal rolling in a dry process and any emissions are expected to go to air (not soil or water). The majority of this airborne IPL is collected and incinerated. Although the equilibrium distribution model predicts that IPL will eventually distribute to soil but equilibrium is unlikely since the emissions during aluminum rolling are to air. In the atmosphere, IPL is expected to be rapidly oxidized via hydroxyl radical attack. Soil could still possibly be a receiving compartment via particulate washout from the atmosphere of un-degraded IPL.

Although air oxidation is expected to be the major fate of IPL emitted to air, biodegradation could also play a role in the fate of any IPL that reaches the soil or water compartments since IPL is expected to be readily biodegradable. The wastewater treatment plant model in EPIWIN estimates 99.98% removal of IPL in a biological treatment system, of which 91.14% is due to biodegradation.

The high log K_{ow} of IPL indicates that it will not be mobile in the soil. The log K_{ow} corresponds to a soil organic matter/water partition coefficient (K_{oc}) value of 4,500. It may be concluded that IPL will not migrate in soil. Applying the principle of equilibrium partitioning, it is also not expected that the bioavailability IPL in soil will be high enough to cause toxicity in soil oganisms.

In summary, the use of IPL in lubricants for metal rolling is expected to result in low emissions to the environment. These emissions would be to air, due to the nature of the process. The major fate of IPL in air is expected to be hydroxyl radical oxidation.

Any IPL that reaches soil or water is expected to be biodegraded so IPL will not persist in the environment. The negligible emissions of IPL and its ease degradation mean that environmental concentrations of IPL will be nil.

8. Environmental effects of released substances:

Environmental studies: Unpublished acute aquatic toxicity studies discussed by Unilever (R. Rodford, 1997, Environmental Safety Laboratory, Unilever Research) resulted in no dose related toxicity in either fish (*Cyprinus carpio*) or *Daphnia magna* when IPL was tested at concentrations above its limit of solubility (dispersed and/or floating, un-dissolved chemical). No data on IPL were found in the Aquire database (US EPA), but isopropyl myrstate was found to have and oral LD_{50} of 47 mg/kg when force-fed to *Cyprinus carpio* (Loeb, 1963).

ASTER does not predict an acute toxic value for IPL due to the fact that its water solubility is less than its expected toxicity. Quantitative structure-activity relationships for acute aquatic toxicity are generally not valid for chemicals with log K_{ow} values above 6. Moreover, it is expected that IPL would be readily metabolized by fish and invertebrates based on the lability of the ester bond. Thus, bioaccumulation in food webs is not expected.

In conclusion, the low water solubility and high log K_{ow} of IPL results in no expected acute toxicity to water or soil dwelling organisms. Furthermore, as developed in section 6, environmental concentrations will be nil. Both the lack of exposure to IPL and its lack of effects mean that the use of IPL in metal rolling lubricants does not pose a risk to the environment.

Mammalian Studies: The available data indicate that isopropyl esters of saturated fatty acids, including IPL, exhibit low toxicity. The LD_{50} of IPL in rats was greater than 5000 mg/kg (EBSI, 1998). These results are similar to that for isopropyl myristate (CIR, 1982b), isopropyl palmitate (CIR, 1982a) and isopropyl sterate (CIR, 1985), which were also nontoxic to rats when administered acutely via the oral route. Isopropyl myristate and isopropyl palmitate were not mutagenic in standard tests for point mutations in bacteria (Blevins and Taylor, 1982). No evidence of systemic toxicity was observed in a subchronic inhalation study using isopropyl myristate (CIR, 1982b). Isopropyl myristate was not carcinogenic in a skin painting study in mice (Stenback and Shubik, 1974).

9. Use of resources and energy

IPL is similar to other surface lubricant additives used to manufacture and process food packaging material and approved under 21 CFR §178.3910, including isopropyl oleate, isobutyl stearate, and methyl esters of fatty acids (C_{16}-C_{18}) derived from animal and vegetable fats and oils. IPL is intended to compete with or replace these substances in surface lubricants. Therefore, there is no effect on the use of natural resources and energy from use of IPL in surface lubricants used in the manufacture of metallic articles.

10. Mitigation measures:

No potential adverse environmental impacts have been identified for the proposed action; therefore, there is no need to discuss mitigation measures.

11. Alternatives to the requested action:

No potential adverse environmental impacts have been identified for the proposed action; therefore, there is no need to discuss alternative to the proposed action.

12. List of preparers

Mr. Larry Gephart, Senior Staff Toxicologist, Exxon Biomedical Sciences Inc. Master in Public Health with Specialization in Toxicology, Board Certified in Toxicology.

Dr. Dennis Peterson, Senior Staff Chemist, Exxon Biomedical Sciences, Inc. PhD. in Biochemistry.

13. Certification:

The undersigned official certifies that the information presented is true, accurate, and complete to the best of the knowledge of Exxon Company International.

2 JUN '99
(Date)

(Signature of responsible official)

14. References

Blevins, R.D. and Taylor, D.E. (1982a). Final report on the safety assessment of octyl palmitate, cetyl palmitate and isopropy palmitate. J. Am. Coll. Toxicol 1(2), 12-35.

CIR (1982b). Final report on the safety assessment of myristyl myristate and isopropyl myristate. J. Am. Coll. Toxicol. 1 (4), 55-80.

CIR (1985). Final report on the safety assessment of butyl sterate, cetyl sterate, isobutyl sterate, isocetyl sterate isopropyl sterate, myristyl sterate, and octyl sterate. J. Am. Coll. Toxicol. 4(5), 107-146.

EBSI (1998). Exxon Biomedical Sciences, Inc. Acute oral toxicity study in the rat, 98MRL 143, Project No. 118102, East Millstone, NJ 08875.

Loeb, H.A. (1963) Acute Oral Toxicity of 1496 Chemicals Force-fed to Carp, US Fish Wildl. Serv., Sp. Sci. Rep.-Fish. No. 471, Washington, D.C.

Mackay, D., A. DiGuardo, S. Patterson and C. Cowan (1996) "Evaluating the Environmental Fate of Chemicals using the EQC model," *Environ. Toxicol. Chem.* 15, 1627-1637. The EQC model is available through Trent University Modeling Centre, http://www.trent.ca/envmodel.

Rodford, R. (1997) *Isopropyl Esters of Saturated Fatty Acids: Safety Evaluation*, Environmental Safety Laboratory, Unilever Research, Doc. Ref. D97/019, Sharnbrook, Bedford, England.

Stenback, F. and Shubik, P. (1974). Lack of toxicity and carcinogenicity of some commonly used cutaneous agents. Toxicol. Appl. Pharmacol. 30, 7.

15. Attachments

Attachment 1: Material Safety Data Sheet for Isopropyl Laurate

MATERIAL SAFETY DATA SHEET

According to ISO 11014

(08-97)

1 Product and company identification

Commercial name	:	ESTOL 1505
Product name	:	Isopropyl laurate
Chemical name	:	
CAS No.	:	10233-13-3
EINECS No.	:	2335601
MITI No.	:	2-798

Company : Unichema North America
4650 South Racine Avenue
Chicago, Illinois 60609
Telefax : 1-773-376-9821
Telephone (24 hour) : 1-773-376-9000
Telephone (Emergency) : CHEMTREC (800) 424-9300

2 Composition/information on ingredients

: Isopropyl ester of lauric acid.
: Not considered as hazardous.
: NFPA Hazard Ratings (Scale 0-4):
Health = 1, Flammability = 1, Reactivity = 0

3 Hazards identification

Health hazards

Inhalation	:	Not applicable at ambient temperature. Vapour from heated product can cause irritation.
Skin contact	:	Unlikely to be irritant.
Eye contact	:	Can cause irritation.
Ingestion	:	Unlikely to be harmful unless excessive amount swallowed.
Physical/chemical hazards	:	None identified
Environmental hazards	:	None identified

4 First-aid measures

Inhalation	:	Remove to fresh air.
Skin contact	:	Wash with plenty of water and soap.
Eye contact	:	Wash well with water without delay and obtain medical attention if any sensations persist.
Ingestion	:	Remove material from mouth. Drink plenty of water. If large amount swallowed or symptoms develop obtain medical attention.

5 Fire-fighting measures

Extinguishing media	: Water (mist), foam, dry powder, carbon dioxide.
Unsuitable extinguishing media	: None
Specific hazards	: Combustion in a restricted volume of air can produce carbon monoxide.
Special protective equipment	: Protective clothing and self-contained breathing equipment should be available for firemen.

6 Accidental release measures

Personal precautions	: No special precautions required.
Environmental precautions	: Minimise contamination of drains, surface and ground waters.
Methods for cleaning up	: Absorb spillage onto inert material (e.g. sand) and collect into suitably labelled containers for disposal at an approved site. Residues and small spillages may be washed away with water and detergent.

7 Handling and storage

Handling	: No special precautions necessary.
Storage	: Store in the original closed containers. Avoid extremes of temperatures.

8 Exposure controls/personal protection

General precautions	: Good industrial hygiene should be followed. Avoid breathing heated vapours.
Ventilation	: Adequate ventilation should be maintained when handling heated product.
Occupational exposure limits	: Not established
Personal protective equipment	: Normal precautions should be observed as for handling all chemicals (chemical safety glasses and protective gloves).

9 Physical and chemical properties

Form/Color/Odor	: Liquid/Colorless/Faint
pH	: Not applicable
Boiling point (10 mbar)	: 145 °C approx.
Cloud point	: -10 °C approx.
Flash point (COC)	: 140 °C approx.
Autoignition temperature	: Not determined
Explosive/ Oxidizing properties	: Not to be expected
Vapour pressure (20 °C)	: <1 mbar
Density (20 °C)	: 850 kg/m^3 approx.
Solubility	: Insoluble in water (20 °C). Soluble in many organic solvents.
Partition coefficient (log Pow) (estimated)	: >3
Viscosity (40 °C)	: 3 mm^2/s approx.
Volatiles	: Not volatile-ambient

10 Stability and reactivity

Stability	: Stable under normal conditions.
Conditions to avoid	: Keep away from heat and flames.
Materials to avoid	: Strong oxidizing agents.
Hazardous decomposition products	: Incomplete combustion can give rise to carbon monoxide.
Hazardous polymerization	: Will not occur.

11 Toxicological information

LD_{50} oral, rat	: >2 g/kg
Skin and eye irritation, rabbit	: Non irritant
Skin sensitization, guinea pig	: No sensitization reactions

12 Ecological information

Degradability	: Readily biodegradable (OECD classification)
LC_0, fish	: >100 mg/l
EC_0, bacteria (Pseudomonas putida)	: >100 mg/l

Based on data for structurally similar substances.

13 Disposal considerations

Waste disposal method	: Recycle where possible. Incinerate according to local regulations.
Contaminated packaging	: Observe local regulations.

14 Transport information

DOT classification	: Not restricted

15 Regulatory information

Classification	: Not hazardous within the meaning of the OSHA Hazard Communication Standard.
SARA hazard	: Title III section 313 - not listed
Inventory status	: Listed on TSCA-CSI (USA), EINECS (EC), DSL (Canada), AICS (Australia) and MITI (Japan).

16 Other information

Literature references	: Isopropyl esters of saturated fatty acids: Safety evaluation Unichema Int., D97/019 (1997).
INCI(CTFA) name	: Isopropyl Laurate